Searching for Drug Information in PubMed

Stereoisomers: Chemicals that have the same molecular formula and sequence of bonds. But they are different chemicals because their atoms are arranged differently in space. When Chemists name stereoisomers they use letters, symbols and prefixes to indicate the specific spatial arrangement of the atoms. But MeSH vocabulary does not get that specific, e.g., both d- and l- Penicillamine are covered under the same MeSH heading Penicillamine. Bottom line when searching, drop the the letters, numbers, symbols, prefixes.

Substance	Search for
d-penicillamine	Penicillamine
l-penicillamine	Penicillamine
dl-tryptophan	Tryptophan
l-tryptophan	Tryptophan
R-pentyl-4-yn-VPA	Valproic Acid
S-pentyl-4-yn-VPA	Valproic Acid
(+)-coronarin E	Coronarin E
(-)-apicularen A	Apicularen A

Salts: When acids and bases react with each other they can form a salt. In MeSH, the preferred term is usually the acid name, not the salt name. Bottom line for searching, try the name of the salt first but check details. If there is no map to MeSH, try the name of the acid.

Salt	Search for
Sodium chloride	Sodium Chloride
potassium sodium tartrate	tartaric acid

aluminum triflate trifluoromethanesulfonic acid

Three useful but confusing subheadings:

Toxicity: **Experimental studies** that explicitly determine the ill effects of the substance.

Poisoning: Life-threatening **intoxication**, which can be accidental, occupational, suicidal, by medication error, or by environmental exposure.

Adverse effects: **Side effects or complications** of a substance used in an accepted dosage when intended for diagnostic, therapeutic, prophylactic, or anesthetic purposes. *Note that this subheading also **includes toxicity and poisoning***.

Registry Numbers (UNIIs, Registry Numbers and Enzyme Commission Numbers)

Unique Ingredient Identifiers (UNIIs) are 10-digit codes assigned by the Food and Drug Administration (FDA) Substance Registration System (SRS) for substances. Registry Numbers (RNs) are assigned by the Chemical Abstracts Service to specific drugs or chemicals. Enzyme Commission (EC) numbers are derived from Enzyme Nomenclature. UNIIs, RNs and ECs are included in the MeSH database records for chemicals, and, when they are available, you can search for them in PubMed. The [rn] search tag is optional. Not all substances have RNs or ECs. NLM currently actively adds UNIIs and ECs, but ceased adding RNs more than 10 years ago. Check the MeSH database to see if one or more of these codes is assigned.

lomerizine [Supplementary Concept]

used to treat migraines

Date introduced: June 11, 1987

Registry Number: DEE37CY4VO

Heading Mapped to:

- Piperazines

Entry Terms:

- KB 2796
- KB-2796
- lomerizine dihydrochloride
- 1-(bis(4-fluorophenyl)methyl)-4-(2,3,4-trimethoxybenzyl)piperazine dihydrochloride

Pharmacologic Action:

- Calcium Channel Blockers

Syntax tips for chemical searches in PubMed:

Syntax Tip #1: Use Quotes only if you must

Search	Details	# of Results
compound 14	compound[All Fields] AND 14[All Fields]	16085
"compound 14"	"compound 14"[All Fields]	196

Syntax Tip #2: Remove brackets and parentheses but keep commas and prime symbols.

There are times when all you have is a chemical name, e.g., 1-[(3,5-dichloro)-2,6-dihydroxy-4-methoxyphenyl]-1-hexanone. When searching systematic names, you need to remove square brackets and open and close parentheses. Square brackets are used to indicate a search field tag in PubMed. Substitute a space, unless there is already a hyphen. Parentheses are interpreted as a nesting operation in PubMed (for example, to nest OR strings), therefore you should *not* include them in your chemical names. Again, substitute a space, unless there is already a hyphen. Hyphens are interpreted as spaces so you can leave them alone.

Systematic name	**Search for**
1-[(3,5-dichloro)-2,6-dihydroxy-4-methoxyphenyl]-1-hexanone	1-3,5-dichloro-2,6-dihydroxy-4-methoxyphenyl-1-hexanone
2,2-(2-chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	2,2-2-chlorophenyl-4'-chlorophenyl-1,1-dichloroethene
1-3,5-dichloro-2,6-dihydroxy-4-methoxyphenyl-1-hexanone	1-3,5-dichloro-2,6-dihydroxy-4-methoxyphenyl-1-hexanone

Syntax tips for chemical searches in PubMed (continued):

Syntax Tip #3:
Try searching the MeSH database using fragments of the compound name

Example: In the MeSH database don't search 2-(2-chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene. Instead try chlorophenyl dichloroethene.